

# 1-[(1H-Benzotriazol-L-yl)methyl]pyridinium

<b>Inchi:</b>	InChI=1S/C12H11N4/c1-4-8-15(9-5-1)10-16-12-7-3-2-6-11(12)13-14-16/h1-9H,10H2/q+1
<b>InchiKey:</b>	NEMINUYEACMXFA-UHFFFAOYSA-N
<b>Formula:</b>	C12H11N4
<b>SMILES:</b>	<chem>c1cc[n+](Cn2nnc3ccccc32)cc1</chem>
<b>Mol. weight [g/mol]:</b>	211.24
<b>CAS:</b>	125713-96-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	1.225		Crippen Method
mcvol	159.330	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C125713964&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C125713964&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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